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Title: Black Box Multigrid Solver for Definite and Indefinite Problems

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Black Box Multigrid Solver for Definite and Indefinite Problems

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Abstract

A two-level analysis method for certain separable problems is introduced. It motivates the definition of improved versions of Black Box Multigrid for diffusion problems with discontinuous coefficients and indefinite Helmholtz equations. For anisotropic problems, it helps in choosing suitable implementations for frequency decomposition multigrid methods. For highly indefinite problems, it provides a way to choose in advance a suitable mesh size for the coarsest grid used. Numerical experiments confirm the analysis and show the advantage of the present methods for several examples.

KEY WORDS elliptic PDEs, discontinuous coefficients, indefinite Helmholyz equations

1 Preliminaries

Consider the nonsingular linear system of equations

$$Ax = b, \tag{1}$$

arising, for example, from a discretization of the elliptic PDE

$$-\nabla(D\nabla u) + \vec{\kappa} \cdot \nabla u + \beta u = f \tag{2}$$

in $\Omega \subset R^d$ with suitable boundary conditions, where d is the dimension of the problem and D, $\vec{\kappa}$ and β are given functions (D is a $d \times d$ symmetric and

uniformly positive definite matrix and $\vec{\kappa}$ is a d-dimensional vector). Assume that A is an operator in $V(\bar{\Omega})$, where $\bar{\Omega} \subset \{\vec{j} = (j_1, \ldots, j_d)\} \subset Z^d$ is the grid and, for any set $g \subset Z^d$, $V(g)$ is the linear space of functions defined on g. With this assumption, A may be considered a tensor $A = (a_{\vec{i},\vec{j}})_{\vec{i},\vec{j} \in \bar{\Omega}}$. In the following, we will treat A both as a matrix and a tensor, assuming that the $\vec{i}$th equation in the matrix A (with some ordering) corresponds to grid point $\vec{i}$. For $1 \leq j \leq d$, denote by $1^{(j)}$ the jth column vector of the identity matrix of order d. Define

$$\partial\bar{\Omega} = \{\vec{i} \in \bar{\Omega} \mid \exists j,\ 1 \leq j \leq d, \text{ such that } \vec{i} + 1^{(j)} \notin \bar{\Omega} \text{ or } \vec{i} - 1^{(j)} \notin \bar{\Omega}\}.$$

When periodic boundary conditions are imposed, Ω and $\bar{\Omega}$ are torus and discrete torus, respectively. Hence in this case $\partial\bar{\Omega} = \emptyset$.

For any set s, let $|s|$ denote its intensity. For any tensor $M = (m_{\vec{i},\vec{j}})$, define the off-diagonal sum operator $r(M)$ by

$$r_{\vec{i}}(M) = \sum_{\vec{j} \in \bar{\Omega}, \vec{j} \neq i} m_{\vec{i},\vec{j}}.$$

1.1 Definition of the Abstract Two-Level Method

Let $\tilde{S} : x \to \tilde{S}x$, $\tilde{S} \equiv \tilde{S}(A, b)$, be a smoothing (relaxation) procedure for (1) with the corresponding iteration matrix S. Let ν_1 and ν_2 be positive integers denoting, respectively, the number of presmoothings and number of postsmoothings used. The operators R (restriction), P (prolongation) and Q (coarse grid coefficient matrix) will be defined later. The abstract two-level (TL) procedure is defined by

$$\text{TL}(x_{in}, A, b, x_{out}): \quad x_{out} = \tilde{S}^{\nu_2}\left(\tilde{S}^{\nu_1} x_{in} + PQ^{-1}R(b - A\tilde{S}^{\nu_1} x_{in})\right). \tag{3}$$

An iterative application of TL is given by

$$\begin{aligned} &x_0 = 0,\ k = 0 \\ &\text{while } \|Ax_k - b\|_2 \geq \text{threshold} \cdot \|Ax_0 - b\|_2 \\ &\quad \text{TL}(x_k, A, b, x_{k+1}) \\ &\quad k \leftarrow k + 1 \\ &\text{endwhile.} \end{aligned} \tag{4}$$

Note that the iteration matrix for this method is

$$S^{\nu_2}(I - PQ^{-1}RA)S^{\nu_1}. \tag{5}$$

This representation is the basis for the two-level analysis in Section 3 below.

1.2 Definition of Black Box Multigrid

Here we describe the Black Box Multigrid method of [5]. It is denoted in the sequel by BBOX.

Assume that A is of 3^d-coefficient stencil, that is,

$$|\vec{i} - \vec{j}|_\infty > 1 \Rightarrow a_{\vec{i},\vec{j}} = 0.$$

For any integer m, denote 'm is even' by $2|m$ and 'm is odd' by $2 \not| m$. For any index set $q \subset \{1, \ldots, d\}$, define the set

$$g(q) = \{\vec{j} \in \bar{\Omega} \mid m \in q \Leftrightarrow 2 \not| \, j_m\}.$$

The family of disjoint sets $\{g(q)\}_{q \subset \{1,\ldots,d\}}$ may be thought of as a coloring of $\bar{\Omega}$ in which the set $g(q)$ corresponds to color q (see [12], Method B). Typically, $g(\emptyset)$ serves as a coarse grid. In the sequel, we will also use the notation $c = g(\emptyset)$ and $f = \bar{\Omega} \setminus c$. This induces a block form for A:

$$A = \begin{pmatrix} A_{ff} & A_{fc} \\ A_{cf} & A_{cc} \end{pmatrix}, \tag{6}$$

where A_{ff} and A_{cc} are of order $|f|$ and $|c|$, respectively.

For any $\vec{i} \in \bar{\Omega}$, let $q(\vec{i}) \subset \{1, \ldots, d\}$ be the set for which $\vec{i} \in g(q(\vec{i}))$. For each $\vec{i} \in f$, define the sets

$$t_{\vec{i}} = \left\{\vec{m} \in \bar{\Omega} \mid \ |\vec{m} - \vec{i}|_\infty \leq 1, \ q(\vec{m}) \subset q(\vec{i})\right\}$$

and, for each $\vec{j} \in t_{\vec{i}}$, the sets

$$s_{\vec{i},\vec{j}} = \left\{\vec{m} \in \bar{\Omega} \mid \ |\vec{m} - \vec{i}|_\infty \leq 1, \ q(\vec{m}) \cap q(\vec{i}) \subset q(\vec{j}) \subset q(\vec{m})\right\}.$$

For $\vec{i} \in c$, define $t_{\vec{i}} = s_{\vec{i},\vec{i}} = \{\vec{i}\}$. In the prolongation, $t_{\vec{i}}$ is the set of grid points contributing to $\vec{i}$ and $s_{\vec{i},\vec{j}}$ is the set of grid points on which a stencil sum ('collapse') is done to compute this contribution. Define the tensors $U = (u_{\vec{i},\vec{j}})$ and $L = (l_{\vec{i},\vec{j}})$ by

$$u_{\vec{i},\vec{j}} = \begin{cases} \sum_{\vec{m} \in s_{\vec{i}\vec{j}}} \tilde{a}_{\vec{i},\vec{m}} & \vec{j} \in t_{\vec{i}} \\ 0 & \text{otherwise} \end{cases} \tag{7}$$

$$\text{and} \quad l_{\vec{i},\vec{j}} = \begin{cases} \sum_{\vec{m} \in s_{\vec{j}\vec{i}}} \tilde{a}_{\vec{m},\vec{j}} & \vec{i} \in t_{\vec{j}}, \ \vec{i} \neq \vec{j} \\ 0 & \text{otherwise,} \end{cases} \tag{8}$$

respectively, where (see [7])

$$\tilde{a}_{\vec{i},\vec{j}} = \begin{cases} -r_{\vec{i}}(A) & \vec{j} = \vec{i} \text{ and } |a_{\vec{i},\vec{i}} + r_{\vec{i}}(A)| \ll |a_{\vec{i},\vec{i}}| \\ a_{\vec{i},\vec{j}} & \text{otherwise.} \end{cases} \tag{9}$$

Assume that the variables are ordered in blocks corresponding to colors q with decreasing order of $|q|$. Since $t_{\vec{i}} \subset \{\vec{i}\} \cup \cup_{|s|<|q(\vec{i})|} g(s)$, U and L are upper and strictly lower triangular matrices, respectively. Define

$$P = U^{-1} diag(U) \text{ and } R = diag(U)(L + diag(U))^{-1}. \tag{10}$$

For symmetric problems, these definitions are equivalent to those of [5]; for nonsymmetric ones, however, they are slightly different from those recommended in [6]. We prefer the present definitions because they allow the simplifications in Section 2.4 below.

For any set $g \subset \bar{\Omega}$, let $J_g : V(\bar{\Omega}) \to V(g)$ be the injection

$$(J_g v)_{\vec{j}} = v_{\vec{j}}, \ v \in V(\bar{\Omega}), \ \vec{j} \in g.$$

The definition of BBOX is completed by

$$\text{either } Q^{-1} = \begin{pmatrix} diag(A_{ff})^{-1}(R_{ff})^{-1} & 0 \\ 0 & (J_c RAP J_c^t)^{-1} \end{pmatrix} \tag{11}$$

$$\text{or } Q^{-1} = \begin{pmatrix} 0 & 0 \\ 0 & (J_c RAP J_c^t)^{-1} \end{pmatrix}. \tag{12}$$

Approach (11) is the one used in [5], whereas (12) is used in [13].

1.3 Difficulties with Black Box Multigrid

We have found in our experiments that Black Box Multigrid has three sources of difficulties:

1. The examples tested in [2] [5] [6] use odd number of grid points in each spatial direction and coarse grids consisting of odd numbered variables of the next finer grid, so that coarse grids always include boundary points. When coarse grids consist of even numbered variables (as for the current implementation) the convergence is somewhat slower.

2. It was pointed out in [13] that Black Box Multigrid stagnates for certain diffusion problems with discontinuous coefficients. This phenomenon is due to strong coupling in the third-level coefficient matrix between subdomains which are only weakly coupled in the original system (see [2]). This strong coupling arises from the collapse (7)–(8) which mixes oblique connections with Cartesian ones, thus introduces strong connections between variables which should be only weakly connected.

3. The performance of Black Box Multigrid deteriorates when (even small) amount of indefiniteness, namely, negative β in (2), is inserted into the equation (by 'Black Box Multigrid' we refer here to the naive, straightforward extension of the method of [5] to indefinite problems (Section 1.2)).

To illustrate the second difficulty, consider Equation (2) in the 2-d region $(0,62)\times(0,62)$ with $\vec{\kappa}\equiv 0$, $\beta\equiv 0$ and $D = diag(\tilde{D},\tilde{D})$, where

$$\tilde{D}(x,y) \;=\; \begin{cases} \frac{1000+1}{2}\cdot\frac{1}{1000} & (x,y)\in\theta\equiv\{(x,y)\mid |x-\omega|+|y-\omega|\le 1\} \\ 1000 & (x,y)\in(0,\omega)\times(0,\omega)\cup(\omega,62)\times(\omega,62)\setminus\theta \\ 1 & (x,y)\in(0,\omega)\times(\omega,62)\cup(\omega,62)\times(0,\omega)\setminus\theta \\ 0 & (x,y)\notin(0,62)\times(0,62), \end{cases}$$

and $0<\omega<62$ is the breaking point. The boundary conditions are

$$\begin{array}{cc} u_n = 0 & x=0 \text{ or } y=0 \\ \tilde{D}u_n + 0.5u = 0 & x=62 \text{ or } y=62. \end{array}$$

The finite volume scheme of [2] is used over an $N\times N$ uniform grid with $N=63$ and the origin lying on the grid point numbered (1,1). The coarse grids consist of even numbered points of the next finer grid (as defined in Section 1.2); this implementation is used throughout the paper, except for certain results in Table 2.1. A four-color Gauss-Seidel smoother ([1] and Method A in [12]) is used in a V(1,1) multigrid cycle. The convergence factor (cf) is defined in (26). It is seen from Table 1.3 that stagnation occurs when the breaking point ω lies on all grids.

Table 1: Convergence factors (cf) for BBOX for diffusion problems with discontinuous coefficients.

ω	levels	(11)	(12)
30	2	.050	.075
30	4	.083	.120
31	2	.067	.096
31	3	.980	.980

2 Improved Versions of Black Box Multigrid

2.1 Improved BBOX for Definite Problems

First we introduce a version which avoids the first difficulty in Section 1.3. Our numerical experiments and the analysis in Section 2.4 suggest that the off-diagonal row-sums $-r_{\vec{i}}(A)$ in (9) should be used only when the prolongation is done along boundaries. This means that one should replace (9) by the following criterion:

$$\tilde{a}_{\vec{i},\vec{j}} = \begin{cases} -r_{\vec{i}}(A) & \vec{j} = \vec{i} \in f \text{ and } t_{\vec{i}} \subset \partial\bar{\Omega} \\ a_{\vec{i},\vec{j}} & \text{otherwise.} \end{cases} \tag{13}$$

Next, we treat the second difficulty of Black Box Multigrid. The algorithm introduced in [10] (also discovered by the authors of [2] in an earlier report) suggests to 'throw' off diagonal elements to the main diagonal; this is done by modifying the $\tilde{a}_{\vec{i},\vec{j}}$'s defined in (13) by

$$\tilde{a}_{\vec{i},\vec{j}} \leftarrow \begin{cases} \tilde{a}_{\vec{i},\vec{i}} + \sum_{\vec{m}\in\bar{\Omega}\setminus t_{\vec{i}}\setminus s_{\vec{i},\vec{i}}} \tilde{a}_{\vec{i},\vec{m}} & \vec{j} = \vec{i} \in f \\ 0 & q(\vec{i}) \setminus q(\vec{j}) \neq \emptyset \neq q(\vec{j}) \setminus q(\vec{i}) \\ \tilde{a}_{\vec{i},\vec{j}} & \text{otherwise} \end{cases}$$

(the main diagonal elements $\tilde{a}_{\vec{i},\vec{i}}$ are modified first). The alternative approach suggested here 'throws' to the main diagonal only elements which are too large to participate in the collapse (7)–(8). Thus, the present version reads as follows. Define

$$\hat{s}_{\vec{i},\vec{j}} = \{\vec{m} \in s_{\vec{i},\vec{j}} \mid |\tilde{a}_{\vec{i},\vec{m}}| \leq \tau |\tilde{a}_{\vec{i},\vec{j}}|\},$$

where $\tau \geq 1$ is a parameter. Do (13) and then, instead of (7)–(8), do

$$u_{\vec{i},\vec{j}} = \begin{cases} \sum_{\vec{m}\in\hat{s}_{\vec{i}\vec{j}}} \tilde{a}_{\vec{i},\vec{m}} & \vec{j} \in t_{\vec{i}},\ j \neq i \\ \sum_{\vec{m}\in\hat{s}_{\vec{i}\vec{i}}} \tilde{a}_{\vec{i},\vec{m}} + \sum_{\vec{k}\in t_{\vec{i}}} \sum_{\vec{m}\in s_{\vec{i}\vec{k}}\setminus\hat{s}_{\vec{i}\vec{k}}} \tilde{a}_{\vec{i},\vec{m}} & \vec{j} = \vec{i} \\ 0 & \text{otherwise,} \end{cases}$$

$$l_{\vec{i},\vec{j}} = \begin{cases} \sum_{\vec{m}\in\hat{s}_{\vec{j}\vec{i}}} \tilde{a}_{\vec{m},\vec{j}} & \vec{i} \in t_{\vec{j}},\ j \neq i \\ 0 & \text{otherwise.} \end{cases}$$

Typically, one should choose τ satisfying

$$1 < \tau < \min_{\vec{i},\ \vec{j}\in\bar{\Omega},\ |a_{\vec{i},\vec{i}}|\geq 4|a_{\vec{j},\vec{j}}|} |a_{\vec{i},\vec{i}}|/|a_{\vec{j},\vec{j}}|.$$

The improved results obtained with $\tau = 10$ for the example in Section 1.3 are displayed in Table 2.1. In our numerical experiments, we also consider

the 'staircase' problem (Example IV in [2]) with a 65×65 grid. For this grid, Criterion (13) suggests that the off-diagonal row-sums $-r_{\vec{i}}(A)$ should not be used on the first level (since the first coarse grid is interior to the finest one) but should be used in coarser levels on the upper and right edges of the discrete boundary, where coarse grid boundary points coincide with fine grid ones. The results in Table 2.1 show the advantage of BBOX with the modified collapse in comparison with the method of [10] (implemented with (11)) (it was also observed that multi level implementations of the method of [10] stagnate for the highly indefinite examples in Section 4).

Table 2: Convergence factors for BBOX with the modified collapse (with $\tau = 10$). For comparison, results for the Kettler–Meijerink method are displayed in the last column.

ω	levels	(11)	(12)	[10]
30	4	.084	.114	.320
31	4	.082	.129	.111
staircase	4	.077	.096	.121

We have also used the above staircase example (again with $N = 65$) to show the advantage of the criterion (13). The coarse grids consist of either even numbered points or odd numbered points of the next finer grid. Note that Criterion (9) corresponds to either the first and third rows in Table 2.1 or the second and fourth ones, depending on the interpretation of the notation '$\ll$' used there. Criterion (13), on the other hand, corresponds to the second and third rows in Table 2.1 (at least on the finest level; the results in the third row can be improved by using Criterion (13) on coarse levels also, see Table 2.1). Thus, it gives optimal results regardless of the construction of coarse grids.

Table 3: Various four-level implementations of BBOX with the modified collapse (with $\tau = 10$) to the staircase problem ($N = 65$).

coarse grids consist of:	$\tilde{a}_{\vec{i},\vec{i}}$	convergence factor
odd numbered points	$a_{\vec{i},\vec{i}}$	.161
odd numbered points	$-r_{\vec{i}}(A)$	.090
even numbered points	$a_{\vec{i},\vec{i}}$	.089
even numbered points	$-r_{\vec{i}}(A)$	.209

2.2 Improved BBOX for Indefinite Problems

The idea is to modify the definition of the restriction and prolongation operators such that the contribution from the term βu in (2) is distributed among spatial directions. To this end, we suggest two possible strategies. The first approach suggests to write $A = G + H$, where H corresponds to a discretization of the term βu in (2). Define the upper triangular matrices $U(G)$ and $U(H)$ by applying (7) to G and H, respectively. Consider the prolongation to a point $\vec{i}$ along certain spatial directions. In order to distribute the contribution from β properly, $U(H)_{\vec{i},\vec{j}}$ should be multiplied by the relative diffusion along these directions, namely,

$$U(H)_{\vec{i},\vec{j}} \leftarrow U(H)_{\vec{i},\vec{j}} \cdot r_{\vec{i}+\vec{e}(\vec{i})}(U(G))/r_{\vec{i}+\vec{e}(\vec{i})}(G),$$

where $\vec{e}(\vec{i}) = 2\vec{g}(\vec{i})$ and $\vec{g}(\vec{i}) \in Z^d$ is the minimal integer vector (in, say, the l_1 norm) for which $\vec{i} + \vec{g}(\vec{i})$ and $\vec{i} + 2\vec{g}(\vec{i})$ are in $\bar{\Omega} \setminus \partial\bar{\Omega}$ ($\vec{e}$ is introduced to avoid the effect of boundary conditions). Alternatively, one can define $\vec{e}(\vec{i}) \equiv 0$ and assume that the matrix argument of the operator $r(\cdot)$ is extended such that its stencil is defined on an infinite grid. P is then obtained by setting $U = U(G) + U(H)$ and proceeding as in Section 1.2. R is defined in a similar way. The lower right block matrix of Q in (11)–(12) is given automatically in the decomposed form $J_c(RGP + RHP)J_c^t$, suitable for recursion in multi-level implementations.

The above definition requires larger storage and set-up time than that of standard BBOX. Furthermore, it requires the a-priori knowledge of the splitting $A = G + H$. Hence, we introduce an alternative approach, which coincides with the previous one for two-level implementations for $(2d+1)$-coefficient stencils for the Helmholtz equation. It reads as follows. Define the discrete β at point $\vec{i}$ by

$$\tilde{\beta}_{\vec{i}} = a_{\vec{i}+\vec{e}(\vec{i}),\vec{i}+\vec{e}(\vec{i})} + r_{\vec{i}+\vec{e}(\vec{i})}(A).$$

Define the relative diffusion at point $\vec{i} \in f$ by

$$d_{\vec{i}} = \frac{\sum_{\vec{j}\in t_{\vec{i}},\ |\vec{i}-\vec{j}|=1} \acute{a}_{\vec{i},\vec{j}}}{\sum_{\vec{j}\in\bar{\Omega},\ |\vec{i}-\vec{j}|_1=1} \acute{a}_{\vec{i},\vec{j}}}.$$

Do (13) and then modify the resulting $\tilde{a}_{\vec{i},\vec{j}}$'s by

$$\tilde{a}_{\vec{i},\vec{j}} \leftarrow \begin{cases} \tilde{a}_{\vec{i},\vec{i}} - \tilde{\beta}_{\vec{i}}\left(1_{\vec{i}} - d_{\vec{i}+\vec{e}(\vec{i})}\right) & \vec{i} = \vec{j} \in f \\ \tilde{a}_{\vec{i},\vec{j}} & \text{otherwise,} \end{cases} \tag{14}$$

where

$$1_{\vec{i}} = \begin{cases} 0 & \vec{i} \in f \text{ and } t_{\vec{i}} \subset \partial\bar{\Omega} \\ 1 & \text{otherwise.} \end{cases}$$

Thus, the contribution of the Helmholtz term βu to main diagonal elements is multiplied by the amount of diffusion in the directions of prolongation (relatively to the total diffusion). (7) and (8) are then used to create P and R and Q is defined as in (11)–(12). This approach works well in practice, e.g., for highly indefinite problems with variable coefficient β and non-rectangular domains. It is denoted hereafter by Averaged Black Box multigrid (ABOX).

2.3 Representations of P for BBOX

For any two sets $t_2 \subset t_1 \subset \{1, \ldots, d\}$, define

$$P_{t_1,t_2} = \begin{cases} -J^t_{g(t_1)} J_{g(t_1)} P^{-1} J^t_{g(t_2)} J_{g(t_2)} & t_1 \neq t_2 \\ 0 & t_1 = t_2. \end{cases}$$

For any ordered set s, let Π_s denote a product of elements indexed in s with a decreasing index order. Then we have

$$P^{-1} = \Pi_{1 \le j \le d} \Pi_{|t_2|=d-j} \Pi_{t_2 \subset t_1} (I - P_{t_1,t_2})$$

and, hence,

$$\begin{aligned} P &= \Pi_{0 \le j \le d-1} \Pi_{|t_2|=j} \Pi_{t_2 \subset t_1} (I + P_{t_1,t_2}) \\ &= I + \sum_{k \ge 2,\ t_1 \subset t_2 \subset \cdots \subset t_k} \Pi_{1 \le l \le k-1} P_{t_{l+1},t_l}. \end{aligned} \tag{15}$$

This representation will be useful in the next section.

2.4 Simplified Representations of P for ABOX

The motivation for the definition of ABOX lies in the opportunity to simplify further the representation of P for schemes involving $(2d+1)$-coefficient stencils, such as finite volume and finite difference schemes. In this case the coefficient matrix A may be written in the form

$$A = \sum_{i=1}^{d} X_i, \tag{16}$$

where X_i represents a three-point discretization of the derivatives in the ith spatial direction (including possible substitution for these derivatives at

boundaries from boundary conditions). It is assumed that the term βu in (2) contributes to $diag(A)$ only; furthermore, it is assumed that the amount of this contribution at point $\vec{i} \in \bar{\Omega}$ is $\tilde{\beta}_{\vec{i}}$, out of which the amount

$$\tilde{\beta}_{\vec{i}} \cdot r_{\vec{i}+\vec{e}(\vec{i})}(X_k)/r_{\vec{i}+\vec{e}(\vec{i})}(A)$$

goes to $(X_k)_{\vec{i},\vec{i}}$ $(1 \le k \le d)$.

Assume also that for each $\vec{i} \in \partial\bar{\Omega}$ and $1 \le j \le d$

$$\left\{\vec{i} + 1^{(j)} \notin \bar{\Omega} \text{ or } \vec{i} - 1^{(j)} \notin \bar{\Omega}\right\} \Rightarrow \vec{i}_j \bmod 2 \in \mathcal{S}_{\vec{i}},$$

where $1^{(j)}$ denotes the jth column vector of the identity matrix of order d and $\mathcal{S}_{\vec{i}}$ is either $\{0\}$ or $\{1\}$. (more accurately, this assumption is required only for directions j for which boundary conditions other than Neumann are imposed). This means that

$$\text{junction points of } \partial\bar{\Omega} \text{ belong to } \; g(\{1,\ldots,d\}) \cup c. \tag{17}$$

With these assumptions, a simple representation of P is available, with which the two-level analysis in Section 3 below is much easier to implement.

For (16), AutoMUG is defined as follows. Let

$$P_i = 2I - diag(X_i)^{-1}X_i \text{ and } R_i = 2I - X_i diag(X_i)^{-1}. \tag{18}$$

Let $\tilde{T}_i$ be the diagonal matrix which has the same row-sums as P_i and define $T_i = \Pi_{j\neq i}\tilde{T}_j$. Define

$$R = J_c\Pi_{1\le j\le d}R_j, \; P = \Pi_{0\le j\le d-1}P_{d-j}J_c^t \text{ and } Q = J_c\sum_{j=1}^{d} T_jR_jX_jP_jJ_c^t. \tag{19}$$

We also consider the Frequency Decomposition Multigrid (FDM) method of [9] for the solution of highly anisotropic equations. When X_i is considerably smaller than all the other X_j's it is suggested in [16] and [9] to use two coarse grid corrections: one with the standard bilinear prolongation and the other with a bilinear-like prolongation but with alternating signs. In [16] the same coarse grid is used for both corrections, whereas in [9] the coarse grid used for the latter correction is shifted so that odd numbered variables are used in the ith spatial direction. This appears to be a considerable improvement (see Table 3.2 below). Here we consider the Child of FDM (CFDM) and the Grandchild of FDM (GFDM) of [8]; these are variants of BBOX (here they are implemented with (13) and (14)) for which 2^d coarse grid corrections are used, each of which uses transfer operators with signs alternating in some of the spatial directions.

For $1 \le i \le d$, define

$$p_i = \{\vec{j} \in \bar{\Omega} \mid 2|j_i\}.$$

Define $\tilde{p}_i = p_i$ for the implementation of [16] and $\tilde{p}_i = \bar{\Omega} \setminus p_i$ for that of [9]. For any set $t \subset \{1, \ldots, d\}$, substitute

$$g(t) \leftarrow (\cap_{i \notin t} \tilde{p}_i) \cap (\cap_{i \in t} (\Omega \setminus \tilde{p}_i))$$

and set $c = g(\emptyset)$ and $f = \bar{\Omega} \setminus c$. Note that this is the same as before for ABOX and for the implementation of [16]. With this redefinition, (15) holds also for the implementation of [9], provided that P is upper triangular when the variables are ordered in blocks $g(t)$ with decreasing order of $|t|$. Define

$$P_i = (I - diag(X_i)^{-1} X_i) J_{p_i}^t J_{p_i} \qquad \text{for ABOX}$$

$$P_i = \begin{cases} \text{(a)} & (I - diag(X_i)^{-1} X_i) J_{p_i}^t J_{p_i} \\ \text{or (b)} & P_i = (diag(X_i)^{-1} X_i - I) J_{\tilde{p}_i}^t J_{\tilde{p}_i} \end{cases} \qquad \text{for CFDM}$$

$$P_i = \begin{cases} \text{(c)} & (I - diag(X_i)^{-1} X_i) J_{p_i}^t J_{p_i} \\ \text{or (d)} & P_i = \Theta_i (diag(X_i)^{-1} X_i - I) J_{\tilde{p}_i}^t J_{\tilde{p}_i} \end{cases} \qquad \text{for GFDM,}$$

where Θ_i is a diagonal matrix measuring the strength of the diffusion in the ith spatial direction: if (d) is used in more than one spatial direction then $\Theta_i = 0$; else,

$$\Theta_i = diag\left(\max\left(0, 1 - (d-1) r_{\vec{j}+\vec{e}(\vec{j})}(X_i) / r_{\vec{j}+\vec{e}(\vec{j})}(A - X_i)\right)\right)_{\vec{j} \in \bar{\Omega}}. \qquad (20)$$

Finally, we consider what we call CFDM(x_i), for which at most two coarse grid corrections are used, namely, Definition (b) is used only when X_i is considerably smaller than all the other X_j's.

With the terminology of Section 2.3, (16) implies that $P_{t_1,t_2} = 0$ if $|t_1 \setminus t_2| \ge 2$. Consequently, (15) obtains the form

$$\begin{aligned} P &= I + \sum_{t \subset \{1,\ldots,d\},\ k \ge 1,\ 1 \le r_1 \ne \cdots \ne r_k \le d,\ r_1,\ldots,r_k \notin t} \Pi_{0 \le l \le k-1} P_{t \cup \{r_1,\ldots,r_{l+1}\}, t \cup \{r_1,\ldots,r_l\}} \\ &= I + \sum_{t \subset \{1,\ldots,d\},\ k \ge 1,\ 1 \le r_1 \ne \cdots \ne r_k \le d,\ r_1,\ldots,r_k \notin t} \\ &\quad \left(\Pi_{0 \le l \le k-1} \left(diag\left(\sum_{i \in t} X_i + \sum_{i=1}^{l+1} X_{r_i} \right) \right)^{-1} diag\left(X_{r_{l+1}} \right) P_{r_{l+1}} \right) J_{g(t)}^t J_{g(t)}. \end{aligned}$$

In the remainder of this paper we consider the implementation (12). Note that for this approach one may substitute

$$P \leftarrow P J_c^t, \quad R \leftarrow J_c R \quad \text{and} \quad Q \leftarrow RAP$$

(in this order). The above equality is then reduced to

$$P = J_c^t + \sum_{k\geq 1,\ 1\leq r_1\neq\cdots\neq r_k\leq d} \left(\Pi_{0\leq l\leq k-1} \left(diag\left(\sum_{i=1}^{l+1} X_{r_i} \right) \right)^{-1} diag\left(X_{r_{l+1}} \right) P_{r_{l+1}} \right) J_c^t.$$

If, in addition, the problem is separable, namely, the $diag(X_i)^{-1}X_i$'s commute with each other, then this simplifies to read (the proof is by induction on d, see [11])

$$\begin{aligned} P &= J_c^t + \sum_{k\geq 1,\ 1\leq r_1<\cdots<r_k\leq d} \left(\Pi_{0\leq l\leq k-1} P_{r_{l+1}} \right) J_c^t \\ &= \Pi_{1\leq i\leq d}(I + P_i) J_c^t. \end{aligned} \tag{21}$$

Note that R also is equal to the right hand side of (21), provided that the multiplication by J_c^t on the right is replaced by a multiplication by J_c on the left and the P_i's are replaced by suitable R_i's. For ABOX, for example, one should use $R_i = J_{p_i}^t J_{p_i}(I - X_i diag(X_i)^{-1})$ and proceed as above, and similarly for the other methods. This gives a uniform representation for ABOX, CFDM, GFDM and AutoMUG and considerably simplifies the two-level analysis introduced next.

3 Two-Level Analysis for Black Box Multigrid

3.1 The Two-Level Analysis Method

Assume that A is diagonalizable and that, for every eigenvector of A of the form $v = \{v_{\vec{j}}\}_{\vec{j}\in\bar{\Omega}}$,

$$v^{(\alpha)} \equiv \{(-1)^{\sum_{i=1}^d \alpha_i j_i} v_{\vec{j}}\}_{\vec{j}\in\bar{\Omega}}, \quad \alpha \in \{0,1\}^d$$

are also eigenvectors of A with the corresponding eigenvalues $\lambda^{(\alpha)}$. This assumption holds, for example, for (a) periodic problems with constant coefficients (namely, when A is a circulant Toeplitz tensor), (b) problems with constant coefficients and 3^d-coefficient stencils and (c) problems of the form (16) (see [17], Sec. 7.1). Let us compute the symbol $\hat{A}$ of A, namely, the representation of A in the subspace spanned by the $v^{(\alpha)}$'s. The basis used for this is $\{J_{g(s)}^t J_{g(s)} v\}_{s\subset\{1,\ldots,d\}}$. For any set s, let 2^s denote the family of subsets of s. Define the isomorphisms

$$\begin{array}{rcccc} s \in 2^{\{1,\ldots,d\}} \to \alpha(s) \in \{0,1\}^d & \text{by} & \alpha(s)_i = 1 & \Leftrightarrow & i \in s \\ \text{and } span\{J_{g(s)}^t J_{g(s)} v\}_{s\subset\{1,\ldots,d\}} \to V(\{0,1\}^d) & \text{by} & J_{g(s)}^t J_{g(s)} v & \to & \alpha(s). \end{array}$$

Then the symbol $\hat{J}_{g(s)}$ is the $(\sum_{i=1}^{d} \alpha(s)_i 2^i + 1)$st row of the identity matrix of order 2^d and $\hat{J}_{p_i} = \sum_{s,\ i \notin s} \hat{J}_{g(s)}$. Define the symmetric orthogonal discrete Haar transform by

$$H = (h_{\gamma,\delta})_{\gamma,\delta \in \{0,1\}^d}, \qquad h_{\gamma,\delta} = 2^{-d/2}(-1)^{\sum_{i=1}^{d} \gamma_i \delta_i}.$$

Then we have

$$\hat{A} = H diag(\lambda^{(\alpha)})_{\alpha \in \{0,1\}^d} H.$$

Clearly, for cases (a) and (b) $\hat{R}$ and $\hat{P}$ are also available. For (16), assume that the X_i's have constant main diagonals and commute with each other. Then the $\hat{X}_i$'s can be computed the same way $\hat{A}$ was and $\hat{R}$ and $\hat{P}$ result from (21) (for GFDM it is also required that the Θ_i's are multiples of the identity). The symbol of Q is then obtained from the symbol product $\hat{Q} = \hat{R}\hat{A}\hat{P}$. For AutoMUG, the symbols of the restriction, prolongation and coarse grid coefficient matrix are computed similarly, using the definitions (18)–(19) and assuming that the matrices $J_c T_i J_c^t$ used there are multiples of the identity (see [11]).

Let $0 \leq k \leq d-1$ be a fixed integer and consider a 2^{d-k}-color hyperplane relaxation with k-dimensional hyperplanes (for example, when $k = 0$ this is a multi-color point relaxation with the colors $g(s)$, $s \subset \{1, \ldots, d\}$). For the symbol $\hat{S}$ of this relaxation, write $\hat{A} = (\hat{A}_{i,j})_{1 \leq i,j \leq 2^{d-k}}$, where the $\hat{A}_{i,j}$'s are blocks of order 2^k corresponding to the various colors. The square matrix symbol of the first color relaxation is then given by

$$\hat{S}_1 = \begin{pmatrix} 0 & -\hat{A}_{1,1}^{-1}\hat{A}_{1,2} & \cdots & -\hat{A}_{1,1}^{-1}\hat{A}_{1,2^{d-k}} \\ 0 & & I & \end{pmatrix}$$

and $\hat{S}$ is just the product of such symbols. The symbol of the iteration matrix (5) is then obtained by replacing individual matrices there by their corresponding symbols. For the multiple coarse grid correction methods CFDM and GFDM, two possible implementations exist: the additive approach, for which the iteration matrix symbol is

$$\hat{S}^{\nu_2} \left(\hat{I} - \left(\sum_j \hat{P}_j \hat{Q}_j^{-1} \hat{R}_j \right) \hat{A} \right) \hat{S}^{\nu_1} \tag{22}$$

(where j runs over all coarse grid corrections) and a multiplicative approach, for which the residual is recomputed after every coarse grid term addition and the iteration matrix symbol is

$$\hat{S}^{\nu_2} \Pi_j (\hat{I} - \hat{P}_j \hat{Q}_j^{-1} \hat{R}_j \hat{A}) \hat{S}^{\nu_1}. \tag{23}$$

The spectrum of the iteration matrix may be computed by scanning over eigenvalues corresponding to elements in a set V of eigenvectors of A satisfying $|V| \geq \lceil |\bar{\Omega}|/2^d \rceil$ and $u, v \in V \Rightarrow u \notin span\{v^{(\alpha)}\}_{\alpha \in \{0,1\}^d}$ and computing numerically the spectra of the corresponding symbols of the iteration matrix.

3.2 Applications

For separable problems of the form (16) the spectrum of A is the sum of those of the tridiagonal matrices X_i. In some cases it is known that these spectra lie in the interior of certain ellipses (or circles, using Gershgorin's theorem) in the complex plane; since the eigenvalues of the iteration matrix are given as a meromorphic function of those of the X_i's, one may scan over the corresponding ellipses (and possible poles of this function) and obtain an upper bound for the asymptotic convergence factor. Alternatively, the spectra of the X_i's can be computed numerically either by an LU method or by a Lanczos type method. Here we apply the two-level analysis method to some model problems for which these spectra are known in advance, namely, Dirichlet problems with constant coefficients in the unit square. The first example is the anisotropic diffusion equation

$$-u_{xx} - \delta u_{yy} = f.$$

with a uniform $N \times N$ grid and the usual five-coefficient second order discretization. The red-black Gauss-Seidel (RB) smoother, (12), (14), $\nu_1 = \nu_2 = 1$ and $N = 63$ are used. It is well-known that for anisotropic problems RB is not an appropriate smoother for single coarse grid correction algorithms. From Table 3.2, however, it can be seen that it is quite efficient in the multiple coarse grid correction algorithms CFDM and GFDM, provided that the implementation of [9] is used. Note that the results for this implementation are only approximations for the actual convergence factors of the methods of [8], since (17) cannot hold for all the coarse grids simultaneously.

Next, we consider indefinite Helmholtz equations. For the slightly indefinite equation

$$-u_{xx} - u_{yy} - 20u = f \tag{24}$$

we obtained spectral radii similar to those for the Poisson equation, namely, .0625 for ABOX and .0741 for AutoMUG. This is in agreement with results in [13] (see Theorem 1 there and the discussion proceeding it). Then we turn to the more difficult highly indefinite equation

$$-u_{xx} - u_{yy} - 790u = f. \tag{25}$$

Table 4: Spectral radii of two-level iteration matrices for an anisotropic diffusion equation with Dirichlet boundary conditions. $N = 63$, the RB smoother and $\nu_1 = \nu_2 = 1$ are used.

δ	residuals	[16]	[16]	[16]	[9]	[9]	[9]
		CFDM(y)	CFDM	GFDM	CFDM(y)	CFDM	GFDM
10^{-2}	not recomputed (22)	.967	.956	.967	.281	.281	.274
10^{-2}	recomputed (23)	.956	.956	.956	.081	.084	.077
10^{-5}	not recomputed (22)	.995	.995	.995	.003	.052	.002
10^{-5}	recomputed (23)	.995	.995	.995	.000	.083	.001

The (scaled) coefficient matrix for this problem with $N = 15$, 31 and 63 has (respectively) 38, 32 and 30 distinct negative eigenvalues, the five smallest (in magnitude) of which are displayed in the 1st, 4th and 7th columns of Table 3.2. This information shows that the problem is nearly singular in the sense of [4]. In the other columns of Table 3.2, the five largest (in magnitude) eigenvalues of the iteration matrices of ABOX and AutoMUG are displayed.

Although the basic iteration (4) diverges, it is seen that for $N = 31$ and $N = 63$ there exist only few isolated eigenvalues of magnitude larger than or close to one. Consequently, it is expected that a Lanczos-type acceleration method applied to (4) will yield suitable linear combinations of iterants in such a way that error components corresponding to large eigenvalues are annihilated. This results in convergence controlled by the small eigenvalues alone, as confirmed numerically in Section 4. Moreover, the analysis in [3] and the multi-level analysis in [13] show that the number of levels may be arbitrarily enlarged, provided that the appropriate mesh-size for the coarsest grid is unchanged. A 31×31 or a 15×15 grid is thus suitable for serving as a coarsest grid in a multi-level implementation for this problem.

4 Numerical Results

The numerical experiments presented here confirm the results of Section 3.2. As a matter of fact, the results in Table 4 coincide with those of Tables 3.2. When acceleration is used, the efficiency of ABOX for highly indefinite problems is shown. Due to its inexpensive multi-level implementation, AutoMUG appears to be competitive in some cases; however, it should be kept in mind that AutoMUG is less robust in the sense that it cannot handle stencils with more than $2d + 1$ coefficients.

Table 5: Five largest negative eigenvalues of A (scaled) and five largest (in magnitude) eigenvalues of two-level iteration matrices for the highly indefinite Helmholtz equation. The RB smoother and $\nu_1 = \nu_2 = 1$ are used.

$N = 15$	$N = 15$	$N = 15$	$N = 31$	$N = 31$	$N = 31$	$N = 63$	$N = 63$	$N = 63$
A	ABOX	AMUG	A	ABOX	AMUG	A	ABOX	AMUG
-0.241	174.13	-886.52	$-1.14\cdot10^{-3}$	-6.710	-17.56	$-1.16\cdot10^{-3}$	-3.409	1.478
-0.368	119.77	-727.10	$-1.90\cdot10^{-2}$	1.680	2.91	$-8.42\cdot10^{-3}$	0.751	-0.928
-0.431	61.56	-594.85	$-2.07\cdot10^{-2}$	1.028	-1.75	$-9.97\cdot10^{-3}$	0.329	0.451
-0.528	-42.44	-511.42	$-5.04\cdot10^{-2}$	-0.700	0.981	$-1.08\cdot10^{-2}$	0.152	-0.183
-0.617	-33.37	-416.42	$-6.03\cdot10^{-2}$	0.554	0.786	$-1.63\cdot10^{-2}$	-0.136	-0.136

We consider Equation (25) with Dirichlet boundary conditions. Although it is ill-posed, it is suitable for serving as a test problem for more realistic situations. It is discretized via a second-order five-point difference scheme on a uniform $N \times N$ grid. The initial guess is random in $(0, 1)$. The solution is $u = 0$. The RB smoother is used in V(0,1) or V(1,1)-cycles. (12) and (14) are used. The second level equation is solved with six orders of magnitude accuracy.

In order to handle iteration matrix eigenvalues of magnitude larger than one, we apply to the basic two-level iteration (4) the Conjugate Gradients Squared (CGS) acceleration method of [14]. We define the following measures of efficiency: the convergence factor

$$\mathrm{cf} = \frac{\|Ax_{last} - b\|_2}{\|Ax_{last-1} - b\|_2} \tag{26}$$

and the preconditioned convergence factor

$$\mathrm{pcf} = \left(\frac{\|\mathcal{P}^{-1}(Ax_{last} - b)\|_2}{\|\mathcal{P}^{-1}(Ax_0 - b)\|_2} \right)^{2/(last\cdot(\nu_1+\nu_2+1))},$$

where $\mathcal{P}$ is the multigrid preconditioner used and $last$ is large enough to realize the process behavior (for pcf, $last$ is the first integer for which the l_2 norm of the preconditioned residual is reduced by six orders of magnitude). The preconditioned residual norm is available in the CGS process; furthermore, since the preconditioned system is better conditioned than the original one, the norm of the preconditioned residual is a better convergence measure than that of the residual itself. It was also checked that the l_2 and l_∞ norms of the

error decrease by at least four orders of magnitude during the convergence process.

The above definition of pcf takes into account the additional work required for smoothing and residual computation; its basic measure is the averaged convergence factor for a V(0,1)-cycle.

In all our tests, we have found essentially no difference between the performances of (11) and (12) for indefinite problems. Since the latter is less expensive in terms of time and storage it was used here. The results are summarized in Tables 4 and 4.

Table 6: Convergence factors (cf) for two-level implementations for the highly indefinite equation. No acceleration is used.

N	ν_1	ν_2	BBOX	AutoMUG	ABOX
31	1	1	10.613	17.563	6.710
63	1	1	2.007	1.478	3.409

Table 7: Preconditioned convergence factors (pcf) for two-level implementations for the highly indefinite equation. CGS acceleration is used.

N	ν_1	ν_2	BBOX	AutoMUG	ABOX
31	1	1	.976	.798	.784
31	0	1	.915	.726	.767

Finally we consider four-level implementations for the slightly indefinite equation (24) with Dirichlet boundary conditions. The RB smoother is used for AutoMUG and a four-color Gauss-Seidel smoother ([1] and Method A in [12]) is used for the other methods. ABOX is implemented with (14). No acceleration is used. The advantage of ABOX and AutoMUG is evident from Table 4. It is also seen that (11) is not better than (12).

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Table 8: Convergence factors (cf) for four-level methods for the slightly indefinite equation. No acceleration is used.

			(11)	(11)	(12)	(12)	
N	ν_1	ν_2	BBOX	ABOX	BBOX	ABOX	AutoMUG
31	1	1	7.196	0.077	7.195	0.063	0.131
63	1	1	0.431	0.064	0.431	0.064	0.096

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